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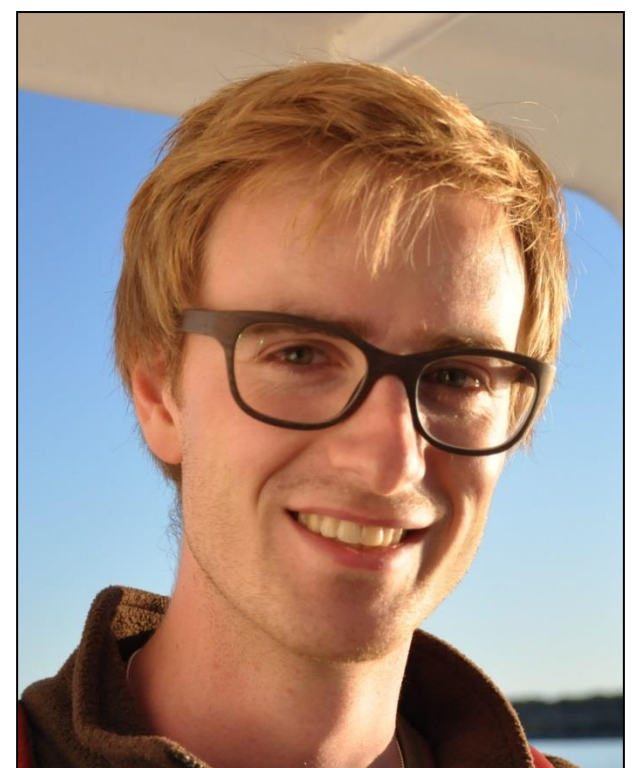
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# The formation dynamics of microbial aggregates

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## Purpose: Why do microbes aggregate?

Microbial granules are aggregates that can contain distinctive structures such as stratified layers or clusters known as micro-colonies. To understand how and why these structures emerge requires knowledge of the ecological forces that govern aggregation.

Large differences in aggregation tendency are observed between different microbial types. In this study we conceptualize different cell-to-cell forces and examine their effect on aggregation. We also show how environmental gradients can favor clustering of different microbial types.

Mechanical agent interactions can be modeled as an interplay between repulsion and attraction resulting from short range forces, such as van der Waals interactions, hydrogen bonds, ionic interactions, as well as longer range hydrophobic interactions.

The magnitude and range of these forces are specific to the model system. iDynoMiCS 2 allows implementation of any force function.

Here, interfacial forces are implemented as linear functions of agent overlap and agent distance. Agents perform a 2D random walk through a periodic domain. The domain is divided in voxels with an initial solute concentrations that changes over time as a function of local consumption and diffusion.

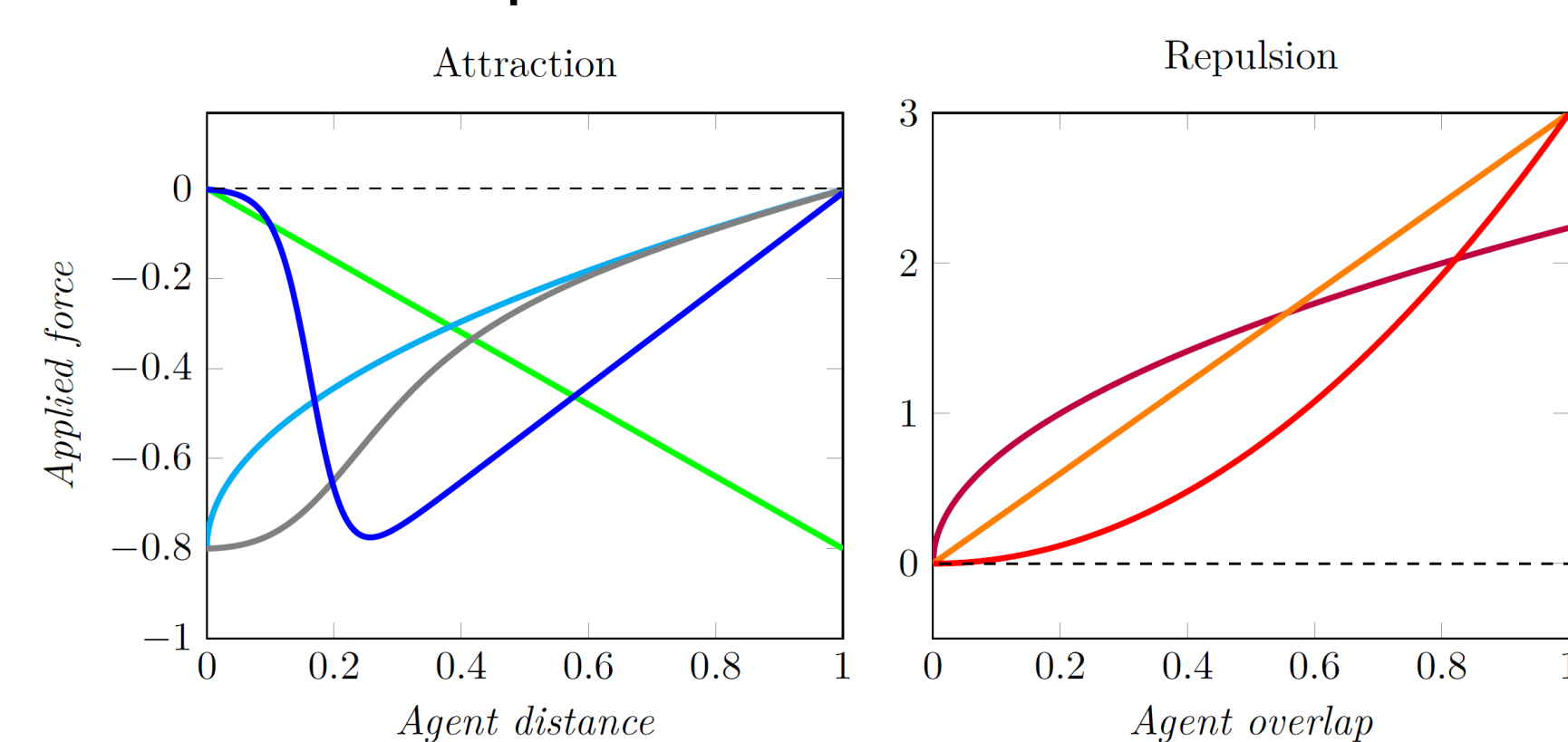


Figure 1: examples of different force functions that can be implemented in iDynoMiCS 2, this study uses a linear force distance relation as shown by the green and orange lines.

## Results: When are types with weak vs strong attachment behavior favored?

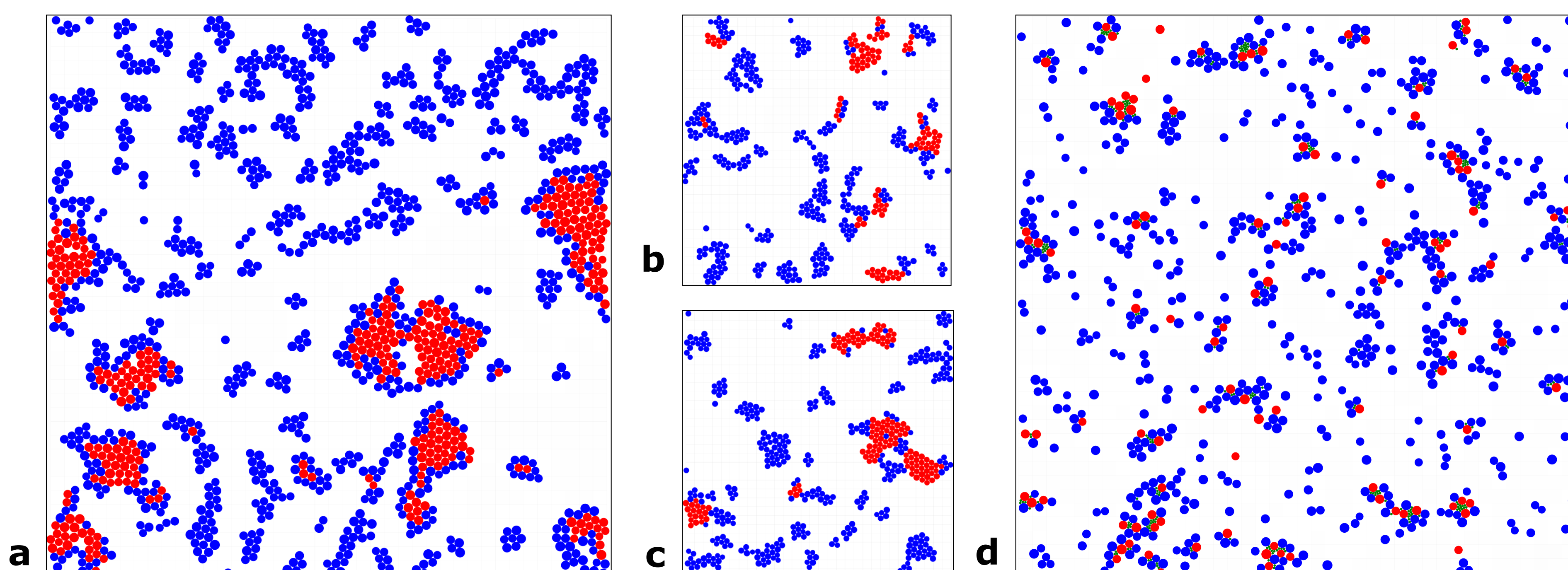


Figure 2: A comparison of different attachment behavior types. Blue and red agents have identical metabolism. Blue agents form weak attachments in all panels. Red agents form strong attachments to any type (a), to siblings only (b), to any other red agents (c), or form EPS particles (green) with strong attachment properties to any agent (d).

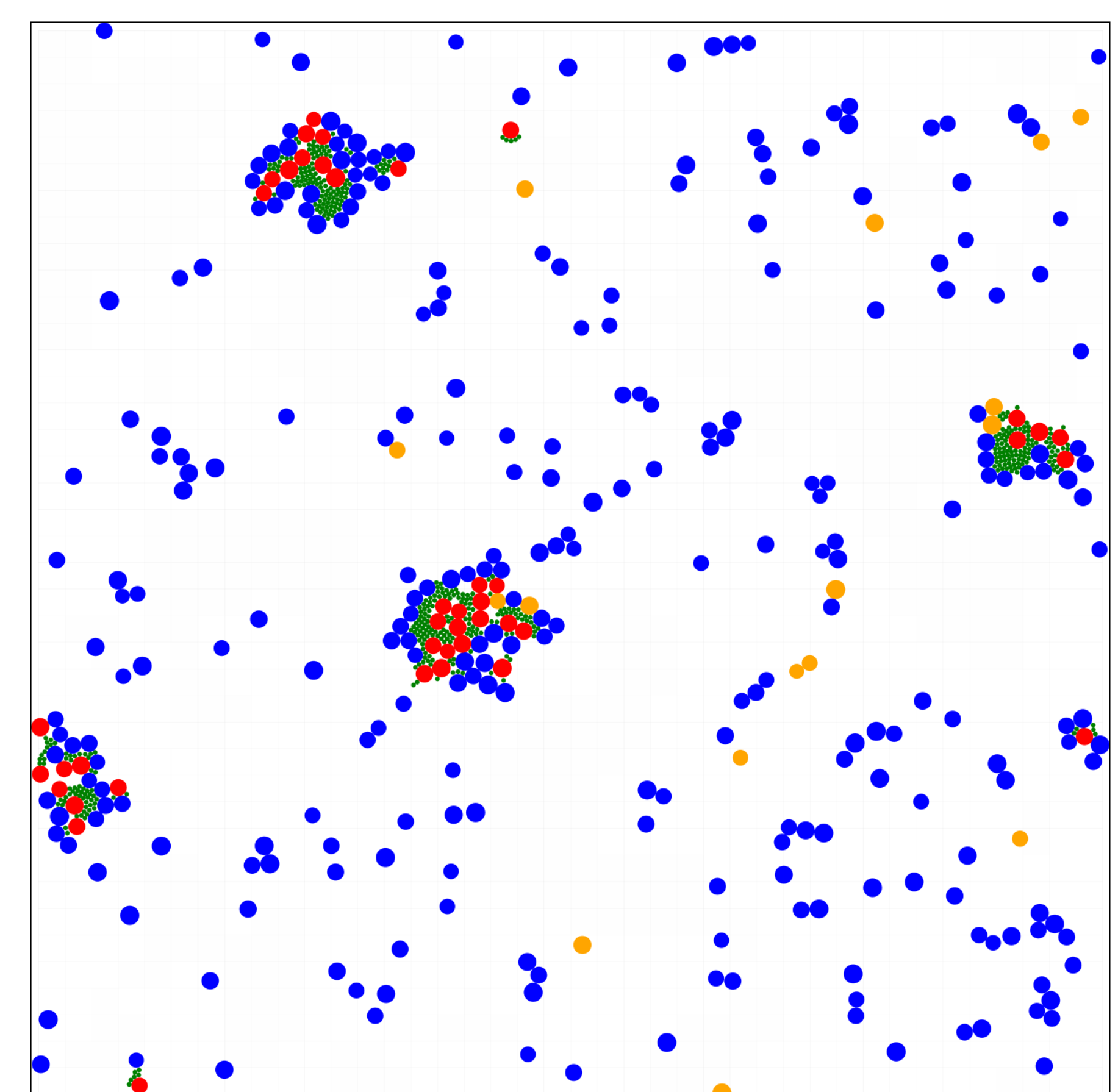


Figure 3: The benefit of aggregation. Blue agents consume solute A, red and orange agents are inhibited by solute A and consume solute B. Red agents also produce EPS particles (green) with strong attachment properties, at a metabolic cost.

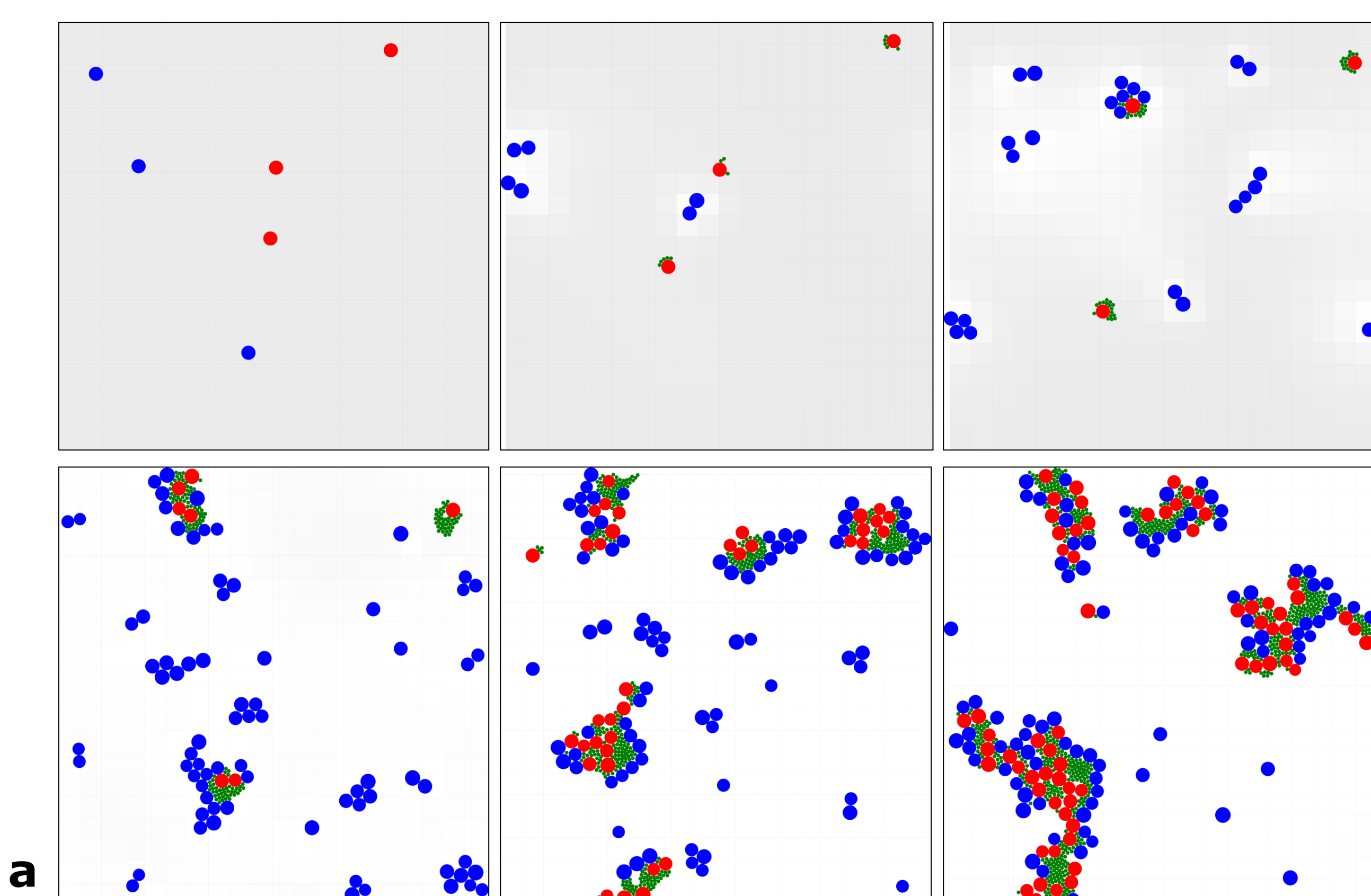


Figure 4: (a) Time series of simulation similar to Fig. 3, without the orange agents with inhibitor concentration shown as gray shading. (b) Detail of simulation showing how the consuming agents lower the local inhibitor concentration to sub-inhibitory levels and growth of the inhibited agent is enabled.

## In conclusion

- In a simple scenario where substrate availability is the only limiting factor, aggregation poses a disadvantage even when the attachment comes at no metabolic cost.
- The formation of a chemical gradient through aggregates can create beneficial niches and thereby a fitness advantage even if the aggregation comes at a metabolic cost.
- Agent based modeling frameworks such as iDynoMiCS 2 are efficient tools to explore and study fitness benefits of individual traits.